

4,4'-Methylenedianiline  
101-77-9 | DTXSID6022422

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

## Model Results

**Predicted value:** 99.6 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 8.93e-01

**Confidence level:** 6.06e-01

## Nearest Neighbors from the Training Set

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4,4'-Methylenedianiline

**Measured:** 92.5

**Predicted:** 99.6

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Benzenamine, 4,4'-(1,2-ethanediyl)bis-

**Measured:** 137

**Predicted:** 114

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(1,1'-Biphenyl)-3,3'-diamine

**Measured:** 93.5

**Predicted:** 89.4

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Benzidine

**Measured:** 120

**Predicted:** 94.2

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2,4'-Biphenyldiamine

**Measured:** 54.5

**Predicted:** 82.7